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A MODIFICATION OF THE NASA PAC 2 CODE TO READ INPUT FROM TAPE.(U)
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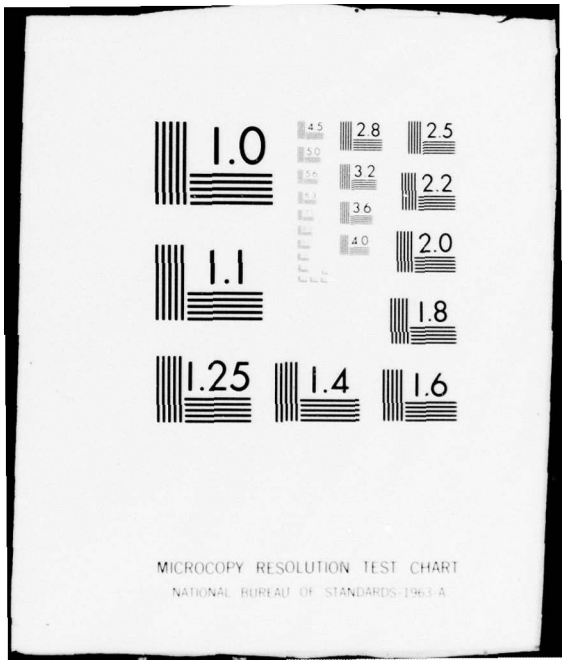
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NWSC/CR/RDTR-81

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A MODIFICATION OF THE NASA PAC 2 CODE TO READ INPUT FROM TAPE

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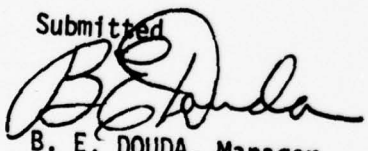

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The NASA Code Fortran IV Program for Calculation of Thermodynamic Data by B. J. McBride and S. Gordon (NASA TN D-4097 dated 1967) has been modified to optionally allow the thermodynamic functions - heat capacity, entropy, and enthalpy - to be read from the magnetic tape of the JANAF Thermochemical Tables furnished by the Dow Chemical Company rather than from cards. The program has also been modified to calculate these thermodynamic functions at the transition points. This previsously had to be done by hand.

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INTRODUCTION

The NASA "PAC 2"[1,2] program for calculation of thermodynamic quantities of chemical species has as one of its options the calculation of heat capacity, enthalpy, and entropy, and the fitting of these to a polynomial function of the temperature. The polynomial coefficients may be specified to be in the form suitable as input data for the companion NASA program to calculate thermodynamic equilibrium.[3] This latter program has found considerable use at NAVWPNSUPPCEN Crane.

In expanding the number of elements which may be involved in the equilibrium program it has been necessary to calculate the polynomial coefficients for many chemical species, using PAC 2.

In order to get accurate polynomial coefficients it is necessary to furnish thermodynamic data at many closely spaced temperatures as input to the PAC 2 program. This involves considerable keypunching. However suitable data for a wide variety of chemical species are in the JANAF tables.[4] Therefore, we have modified PAC 2 to read the data from the JANAF tape rather than from cards.

Another time-saving modification was related to the requirement of the PAC 2 program for input data at the transition points. This is not available in the JANAF tables, and it had been necessary to obtain it by hand calculation. The modified program now does this by extrapolation from the other data furnished.

GENERAL DESCRIPTION OF PROGRAM

The PAC 2 program has options for a number of different types of functions to be calculated. In a particular run a list of species may be given, with a different option requested for each. For any particular species a variety of methods are available, each requiring a different type of input data.

Typically, using the JANAF tables[4] as a data source, one would read in the thermodynamic functions at 100 degree intervals for the solid and some of the liquid phases using the READIN method. For liquid phases where the heat capacity is given as constant, or can readily be seen to

be a linear function of temperature, it is most efficient to furnish this information and use the COEF method. For gaseous species one of the theoretical methods (JANAF, PANDK, etc.) using spectroscopic data required the least effort in preparing input.

The new option was designed to take the thermodynamic data from the magnetic tape using the READIN method, and then use the LSTSQS option to obtain the polynomial coefficients. It is probably possible to change options and methods from one species to the next during a given run since the other options and methods were not changed. This was specifically demonstrated using the JANAF method to generate the polynomial temperature coefficients of the thermodynamic functions for one species in a list, while using READIN from tape for the others. It is also possible to turn off the tape and furnish the input for the READIN method from cards for arbitrary species within a list. It is not possible to switch between tape and cards as input for the READIN method for different phases of a particular species. It is also not possible to change methods on going from one phase to the next with the tape on option, for instance to use READIN for the solid phases, then use COEF for the liquid phase. However, this change of method can still be done if READIN is performed using data from cards, with TAPEOFF specified.

Despite this latter restriction, the simplification of the preparation of input for reading data from tape more than compensates for the extra computer time involved in doing least squares fits to phases with constant heat capacities.

SPECIFIC INPUT CARDS

The cards to be used for each species, with changes made from the PAC 2 program as described in references 1 and 2, are as follows:

1. Formula Card - no change from reference 1.
2. TAPEOFF Card - requires the data to be read from cards. In the absence of this card data are read from the tape.
3. LSTSQS - no change from reference 1.
4. Method Card - contains melting point or transition temperature and heat of transition, as in reference 1. The only change

is that at a melting point, but not at other phase transitions, the new heat of formation must be provided, since subsequent data from the tape are relative to it.

5. Data Card - a single card gives the species number (see a listing of the JANAF data tape) and the temperature range, in even hundreds, for the new phase, in 3I4 format. The method and data cards are repeated for each phase, as in reference 1.

6. Finish Card - as in reference 1.

OPERATION OF THE MODIFIED PROGRAM

Upon reading the data card the program searches the data tape for the species number given, and there reads C_p, S, and $H-H_{298}$ data at each 100 degree interval between the limits given on the data card. The next input card is then read, giving the next transition temperature. The program then computes the polynomial coefficients by the least squares procedure; and these coefficients are then used to calculate the thermodynamic functions C_p, S, and $H-H_{298}$ for the low temperature phase at the transition temperature. The enthalpy of transition is then used to calculate the enthalpy and entropy for the high temperature phase at this transition.

The next data input card is read, and the program then selects from the data tape the values of C_p, S, and $H-H_{298}$ above the transition. In the case the transition is a melting point, the new $H-H_{298}$ data are corrected to refer to the heat of formation of the solid at 298.15^{o}. The heat capacity of the high temperature phase at the transition is then obtained by backward extrapolation from the succeeding 1 to 3 (as available) values of C_p . The program now has all the data needed for the least squares procedure to evaluate the polynomial coefficients for this phase. The procedure is repeated until all requested phases have been calculated.

The input information from cards and tapes, and the smoothed values, are printed. The polynomial coefficients are put onto a punch tape in the format required for the data input cards of reference 3. This is just as is done in reference 1. The data calculated for the transition temperature are included in the printout.

REFERENCES

1. B. J. McBride and S. Gordon, "Fortran IV Program for Calculation of Thermodynamic Data", NASA TN D-4097, National Aeronautics and Space Administration, Lewis Research Center, Cleveland, OH (August 1967). Available N67-35192. National Technical Information Service.

2. Informal communication regarding a modification, PAC 2, to the computer program of reference 1 (April 1972).

3. S. Gordon and B. J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations", NASA SP-273, Lewis Research Center (1971). Available NTIS-N71-37775.

4. "JANAF Thermochemical Tables", NSRDS-NBS 37, The Thermal Research Laboratory, Dow Chemical Co., Midland, MI (June 1971). Available U.S. Government Printing Office, Washington, D.C. 20402, Catalog No. C 13.48:37. Loose leaf supplements and magnetic tape available from the Thermal Research Laboratory, Dow Chemical Co., Midland, MI 48640.

APPENDIX A

New Variables

ASDH	Correction term to ASINDH for new phase
CHS	Contents of a card
DD	Array of thermodynamic functions from tape
ICODE	Code number of current species
IFIRST	Next tape access will be the first for this species
IJW	Buffer area
IKODE	Code number on card from tape
IOLDC	Code number of last species obtained from tape
ITAPE	Number of temperatures selected from tape for input to the least squares routine
NFRST	Flag to indicate that this is the first card for the current species
NREC	Number of temperatures read from tape
PHASDW	Increment in enthalpy at phase transition
PHAST	Phase transition temperature
POLTU	Lower temperature limit for previous polynomial
POLTUL	Upper temperature limit for previous polynomial
TAPE8	Logical file name for thermodynamic data tape
TEST (2)	Input thermodynamic data from tape (if true)
TLAGR	Perform a Lagrangian interpolation (if true)
TLL	Lower temperature limit for data to be selected
TUL	Upper temperature limit for data to be selected
TT	Array of temperatures from tape
TTON	Thermodynamic data is to be read from tape (if true)

APPENDIX B
PROGRAM CHANGES

PRINTOUT FROM UPDATE ROUTINE

UNLABELED OLDPL IDENT CHANGE UPDATE 1.2-78186. 10/30/78 09.13.07. PAGE 1

```
*****    *IDENT CHANGE
*****    *DELETE MAIN.3
              1TAPE7=PUNCH,TAPE4,TAPE3,TAPE8,TAPE9)
*****    *INSERT MAIN.5
         C     TEST(2)  INPUT FROM TAPE
*****    *DELETE MAIN.24
              LOGICAL TEST,IFIRST,TTON
*****    *INSERT MAIN.26
              COMMON /TAP/IJW(800),TT(100),DD(100,7),CMS(80),NREC,IFIRST
*****    *DELETE MAIN.35
              1 *ORD(4),D(4),NAM(4),ITAPE
*****    *DELETE MAIN.37
              1  NLAST, POLTLL, POLTUL
*****    *INSERT MAIN.50
              DATA I4BLNK/4H    /
*****    *DELETE MAIN.66
              DO 109 I=2,20
*****    *DELETE MAIN.68
*****    *DELETE MAIN.69
              TTON = .TRUE.
              LDATE(1) = I4BLNK
              LDATE(2) = I4BLNK
*****    *INSERT MAIN.90
              CPR(I) = 0.0
              MHRT(I) = 0.0
              FHRT(I) = 0.0
*****    *INSERT MAIN.104
              IF(ICARD.EQ.4HTAPE) GO TO 132
*****    *INSERT MAIN.116
              IFIRST = .TRUE.
*****    *INSERT MAIN.215
              TEST(2) = .TRUE.
              IF(.NOT.TTON) TEST(2) = .FALSE.
*****    *INSERT MAIN.291
         C
         C    SET FLAG TO TURN TAPE ON OR OFF FOR THE READIN METHOD ONLY.
           132 IF(ICARD2.EQ.2HOF) TTON = .FALSE.
              IF(ICARD2.EQ.2HON) TTON = .TRUE.
              GO TO 104
*****    *DELETE INPUT.12
             1WORD(4),D(4),NAM(4),ITAPE
*****    *INSERT INPUT.19
              IF (TEST(2)) GO TO 500
           101 TEST (2) = .FALSE.
*****    *INSERT INPUT.22
           400 WRITE(4,10)ICARD,ICARD2,((AWD(J,I),J=1,6),(FWD(K,I),K=1,12),
*****    *DELETE INPUT.23
*****    *INSERT INPUT.24
              BACKSPACE 4
              GO TO 310
           500 IF (ITAPE.EQ.0) GO TO 101
              ITAPE = ITAPE - 1
           310 READ(4,10)ICARD,ICARD2,((AWD(J,I),J=1,6),(FWD(K,I),K=1,12),I=1,4),
             1 IWORD(5)
              BACKSPACE 4
```

```
*****    *DELETE INPUT.28
           600 IF (ICARD.NE.IEFDA) GO TO 14
*****    *DELETE INPUT.38
*****    *INSERT INPUT.41
               BACKSPACE 4
               GO TO 1000
*****    *DELETE INPUT.42
*****    *DELETE INPUT.118
*****    *DELETE TEMPER.11
*****    *INSERT TEMPER.12
               DATA IT/1HT/,I/1HI/,IBLANK/1H /
*****    *INSERT TEMPER.68
               IWORD(4)=IBLANK
               WORD(4)=0.0
*****    *DELETE RECO.6
               LOGICAL TEST, TSTRED, TSTCO, TSTK, TLAGR
*****    *INSERT RECO.16
               COMMON /PCH/LEVEL,NF1,NF2,C(9,15),TC(10), NTC,NEX,LDATE(2),NNN
              1  ,NLAST, POLTLL, POLTUL
*****    *DELETE RECO.29,RECO.30
             9  ,IASH/4HASIN/
*****    *INSERT RECO.35
               PHASDH = 0.0
               PHAST = IT
               TLAGR = .FALSE.
               ASDH = 0.0
*****    *DELETE RECO.49
               IF(IWORD(I).EQ.IASH) GO TO 41
                IF (IWORD(I).NE.ICOEF) GO TO 16
               TSTCO = .TRUE.
               TEST (2) = .FALSE.
            16 IF (IWORD(I).EQ.KCAL) TSTK=.TRUE.
*****    *DELETE RECO.50
*****    *INSERT RECO.55
               IF(IWORD(I).EQ.IT) PHAST = WORD(I)
*****    *INSERT RECO.67
               PHASDH = WORD(I)
               GO TO 2200
            41 CONTINUE
               ASDH = (WORD(I) - ASINDH)/R
*****    *INSERT RECO.68
               PHASDH = PHASDH/R/PHAST
*****    *INSERT RECO.80
               IF(.NOT.TEST(2)) GO TO 45
               NT = NT + 1
               T(NT) = PHAST
               NTT = NT + 1
               NIT = NTT
      C
      C    CALCULATE FUNCTIONS FOR THE FIRST POINT AFTER A PHASE TRANSITION
      C    USING THE POLYNOMIALS FROM THE PREVIOUS PHASE AND DELTAH.
      C   STORE FUNCTIONS AT NNN.
      C
               TLAGR = .TRUE.
               NLAGR = 0
```

```
            IROW = 1
            IF(POLTUL.GT.1000.) IROW = 2
            CPR(NNN) = 0.0
            FC1 = 0.0
            HHRT(NNN) = C(IROW,6)/PHAST + PHASDH - ASINDH/R/PHAST
            FC3 = C(IROW,7) + PHASDH
            DO 32 I=1,NF
            TP = PHAST**EX(I)
            IF(EX(I).NE.-1.0) GO TO 37
            HHRT(NNN) = HHRT(NNN) + C(IROW,I)*ALOG(PHAST)/PHAST
            GO TO 38
         37 HHRT(NNN) = HHRT(NNN) + C(IROW,I)*TP/(EX(I)+1.0)
            IF(EX(I).NE.0) GO TO 38
            FC3 = FC3 + C(IROW,I)*ALOG(PHAST)
            GO TO 32
         38 FC3 = FC3 + C(IROW,I)*TP/EX(I)
         32 FC1 = FC1 + C(IROW,I)*TP
            FHRT(NNN) = FC3 - HHRT(NNN)
         45 CONTINUE
*****    *INSERT RECO.91
            IF (TEST(2)) CALL TAPEIN(LINES)
*****    *DELETE RECO.105
            IOUT = IBLNK
*****    *DELETE RECO.157
*****    *INSERT RECO.159
            HHRT(NTT) = HHRT(NTT) + ASDH/TT
*****    *INSERT RECO.215
C
C     CALCULATE CP/R FOR FIRST POINT AFTER PHASE TRANSITION USING UP TO A
C     THREE POINT LAGRANGIAN INTERPOLATION WITH THE SECOND PHASE DATA.
C
            IF(.NOT.TEST(2)) GO TO 34
            IF(.NOT.TLAGR) GO TO 34
            NLAGR = NLAGR + 1
            IF(NLAGR.EQ.1) TCONST = PHAST
            IF(NLAGR.EQ.1) CPR(NNN) = CPR(NTT)
            IF(NLAGR.LT.2.OR.NLAGR.GT.3) GO TO 34
            CPR(NNN) = 0.0
            DO 35 K=1,NLAGR
            BK = 1.0
            NDEXK = NT - NLAGR + K
            DO 36 J=1,NLAGR
            IF(J.EQ.K) GO TO 36
            NDEXJ = NT - NLAGR + J
            BK = BK*((PHAST-T(NDEXJ))/(T(NDEXK)-T(NDEXJ)))
         36 CONTINUE
            NDEXK = NTT-NLAGR + K
            CPR(NNN) = CPR(NNN) + BK*CPR(NDEXK)
         35 CONTINUE
         34 CONTINUE
*****    *INSERT ATOM.19
            LOGICAL TEST,TSTFIL,GLABEL
            EQUIVALENCE (Q,AJ),(TAPE,TDQDT)
*****    *DELETE ATOM.22,ATOM.23
*****    *INSERT LINK1.31
```

```
      EQUIVALENCE (TAPE,SQ)
***** *DELETE LINK1.37
***** *INSERT DERIV.5
      DIMENSION I(5), J(6)
***** *DELETE DERIV.14
***** *INSERT LEAST.123
      NFP=NF
***** *INSERT LEAST.147
      NPTS=NEND-NBEGIN+1
      NF=NFP
      IF(NPTS.GE.NF) GO TO 47
      NF=NPTS
   47 NF1=NF+1
      NF2=NF+2
      NF3=NF+3
      NF4=NF+4
      NF5=NF+5
      NF6=NF+6
      DO 49 I=NF1,NFP
   49 ANS(ILOW,I)=0.
***** *DELETE LEAST.234
***** *DELETE LEAST.247
***** *DELETE LEAST.293
  580 DO 581 I=1,NF
***** *INSERT LEAST.294
      NFP1=NFP+1
      NFP2=NFP+2
      ANS(ILOW,NFP1)=ANSTPY(NF1)
      ANS(ILOW,NFP2)=ANSTPY(NF2)
***** *DELETE LEAST.444
      NF1=NFP1
      NF2=NFP2
***** *INSERT LEAST.450
      NF = NFP
***** *DELETE PUNCH.19
     1  NLAST, POLTLL, POLTUL
***** *INSERT PUNCH.76
      POLTLL = DAT4
      POLTUL = DAT5
***** *ADDFILE
***** *DECK TAPIN
```

INPUT

MODIFICATIONS / CONTROL CARDS

```
MAIN          1TAPE7=PUNCH,TAPE4,TAPE3)
MAIN          1TAPE7=PUNCH,TAPE4,TAPE3,TAPE8,TAPE9)
MAIN     C     TEST(2)  INPUT FROM TAPE
MAIN          LOGICAL TEST
MAIN          LOGICAL TEST,IFIRST,TTON
```

```
                MAIN      3      D
                CHANGE    1      I
                CHANGE    2      I
PAC10032        MAIN     24      D
                CHANGE    3      I
```

```
MAIN          COMMON /TAP/IJW(800),TT(100),DD(100,7),CMS(80),NREC,IFIRST                CHANGE     4      I
MAIN         1 WORD(4),D(4),NAM(4)                                                      MAIN      35        D
MAIN         1 WORD(4),D(4),NAM(4),ITAPE                                                CHANGE     5      I
MAIN         1       NLAST                                                              MAIN      37        D
MAIN         1  NLAST, POLTLL, POLTUL                                                   CHANGE     6      I
MAIN          DATA I4BLNK/4H    /                                                       CHANGE     7      I
MAIN          DO 109  I = 3,20                                          PAC10056      MAIN      66        D
MAIN          DO 109 I=2,20                                                           CHANGE     8      I
MAIN          LDATE(1) = 0                                                            MAIN      68        D
MAIN          LDATE(2) = 0                                                            MAIN      69        D
MAIN          TTON = .TRUE.                                                           CHANGE     9      I
MAIN          LDATE(1) = I4BLNK                                                       CHANGE    10      I
MAIN          LDATE(2) = I4BLNK                                                       CHANGE    11      I
MAIN          CPR(I) = 0.0                                                            CHANGE    12      I
MAIN          HHRT(I) = 0.0                                                           CHANGE    13      I
MAIN          FHRT(I) = 0.0                                                           CHANGE    14      I
MAIN          IF(ICARD.EQ.4HTAPE) GO TO 132                                           CHANGE    15      I
MAIN          IFIRST = .TRUE.                                                         CHANGE    16      I
MAIN          TEST(2) = .TRUE.                                                        CHANGE    17      I
MAIN          IF(.NOT.TTON) TEST(2) = .FALSE.                                         CHANGE    18      I
MAIN     C                                                                            CHANGE    19      I
MAIN     C   SET FLAG TO TURN TAPE ON OR OFF FOR THE READIN METHOD ONLY.              CHANGE    20      I
MAIN       132 IF(ICARD2.EQ.2HOF) TTON = .FALSE.                                     CHANGE    21      I
MAIN           IF(ICARD2.EQ.2HON) TTON = .TRUE.                                      CHANGE    22      I
MAIN           GO TO 104                                                             CHANGE    23      I

17

INPUT          1 WORD(4),D(4),NAM(4)                                                  INPUT     12        D
INPUT         1WORD(4),D(4),NAM(4),ITAPE                                              CHANGE    24      I
INPUT          IF (TEST(2)) GO TO 500                                                CHANGE    25      I
INPUT       101 TEST (2) = .FALSE.                                                   CHANGE    26      I
INPUT       400 WRITE(4,10)ICARD,ICARD2,((AWD(J,I),J=1,6),(FWD(K,I),K=1,12),         CHANGE    27      I
INPUT           WRITE(4,10)ICARD,ICARD2,((AWD(J,I),J=1,6),(FWD(K,I),K=1,12),         INPUT     23        D
INPUT           BACKSPACE 4                                                           CHANGE    28      I
INPUT           GO TO 310                                                             CHANGE    29      I
INPUT       500 IF (ITAPE.EQ.0) GO TO 101                                             CHANGE    30      I
INPUT           ITAPE = ITAPE - 1                                                     CHANGE    31      I
INPUT       310 READ(4,10)ICARD,ICARD2,((AWD(J,I),J=1,6),(FWD(K,I),K=1,12),I=1,4),    CHANGE    32      I
INPUT          1 IWORD(5)                                                           CHANGE    33      I
INPUT           BACKSPACE 4                                                           CHANGE    34      I
INPUT           IF (ICARD.NE.IEFDA) GO TO14                                           INPUT     28        D
INPUT       600 IF (ICARD.NE.IEFDA) GO TO 14                                          CHANGE    35      I
INPUT           BACKSPACE 4                                                           INPUT     38        D
INPUT           BACKSPACE 4                                                           CHANGE    36      I
INPUT           GO TO 1000                                                            CHANGE    37      I
INPUT           GO TO 310                                                             INPUT     42        D
INPUT       310 BACKSPACE 4                                                           INPUT    118        D


TEMPER          DATA IT/1HT/,I/1HI/,IBLANK/1H /                           TEMP0005      TEMPER    11        D
TEMPER          DATA IT/1HT/,I/1HI/,IBLANK/1H /                                         CHANGE    38      I
TEMPER          IWORD(4)=IBLANK                                                         CHANGE    39      I
TEMPER          WORD(4)=0.0                                                             CHANGE    40      I
```

```
RECO          LOGICAL TEST, TSTRED, TSTCO, TSTK                                    RECO        6        D
RECO          LOGICAL TEST, TSTRED, TSTCO, TSTK, TLAGR                             CHANGE     41     I
RECO          COMMON /PCH/LEVEL,NF1,NF2,C(9,15),TC(10), NTC,NEX,LDATE(2),NNN       CHANGE     42     I
RECO         1  ,NLAST, POLTLL, POLTUL                                            CHANGE     43     I
RECO          COMMON /PCH/LEVEL,NF1,NF2,C(9,15),TC(10), NTC,NEX,LDATE(2),NNN       RECO       29       D
RECO         1 ,NLAST                                                             RECO       30       D
RECO         9  ,IASH/4HASIN/                                                     CHANGE     44     I
RECO          PHASDH = 0.0                                                        CHANGE     45     I
RECO          PHAST = TT                                                          CHANGE     46     I
RECO          TLAGR = .FALSE.                                                     CHANGE     47     I
RECO          ASDH = 0.0                                                          CHANGE     48     I
RECO          IF (IWORD(I).EQ.ICOEF) TSTCO = .TRUE.                  REC00049 RECO       49       D
RECO          IF(IWORD(I).EQ.IASH) GO TO 41                                       CHANGE     49     I
RECO           IF (IWORD(I).NE.ICOEF) GO TO 16                                    CHANGE     50     I
RECO          TSTCO = .TRUE.                                                      CHANGE     51     I
RECO          TEST (2) = .FALSE.                                                  CHANGE     52     I
RECO        16 IF (IWORD(I).EQ.KCAL) TSTK=.TRUE.                                 CHANGE     53     I
RECO          IF(IWORD(I).EQ.KCAL) TSTK=.TRUE.                                    RECO       50       D
RECO          IF(IWORD(I).EQ.IT) PHAST = WORD(I)                                  CHANGE     54     I
RECO          PHASDH = WORD(I)                                                    CHANGE     55     I
RECO          GO TO 2200                                                          CHANGE     56     I
RECO        41 CONTINUE                                                           CHANGE     57     I
RECO          ASDH = (WORD(I) - ASINDH)/R                                         CHANGE     58     I
RECO          PHASDH = PHASDH/R/PHAST                                             CHANGE     59     I
RECO          IF(.NOT.TEST(2)) GO TO 45                                           CHANGE     60     I
RECO          NT = NT + 1                                                         CHANGE     61     I
RECO          T(NT) = PHAST                                                       CHANGE     62     I
RECO          NTT = NT + 1                                                        CHANGE     63     I
RECO          NIT = NTT                                                           CHANGE     64     I
RECO     C                                                                        CHANGE     65     I
RECO     C    CALCULATE FUNCTIONS FOR THE FIRST POINT AFTER A PHASE TRANSITION    CHANGE     66     I
RECO     C    USING THE POLYNOMIALS FROM THE PREVIOUS PHASE AND DELTAH.           CHANGE     67     I
RECO     C   STORE FUNCTIONS AT NNN.                                             CHANGE     68     I
RECO     C                                                                        CHANGE     69     I
RECO          TLAGR = .TRUE.                                                      CHANGE     70     I
RECO          NLAGR = 0                                                           CHANGE     71     I
RECO          IROW = 1                                                            CHANGE     72     I
RECO          IF(POLTUL.GT.1000.) IROW = 2                                        CHANGE     73     I
RECO          CPR(NNN) = 0.0                                                      CHANGE     74     I
RECO          FC1 = 0.0                                                           CHANGE     75     I
RECO          HHRT(NNN) = C(IROW,6)/PHAST + PHASDH - ASINDH/R/PHAST               CHANGE     76     I
RECO          FC3 = C(IROW,7) + PHASDH                                            CHANGE     77     I
RECO          DO 32 I=1,NF                                                        CHANGE     78     I
RECO          TP = PHAST**EX(I)                                                   CHANGE     79     I
RECO          IF(EX(I).NE.-1.0) GO TO 37                                          CHANGE     80     I
RECO          HHRT(NNN) = HHRT(NNN) + C(IROW,I)*ALOG(PHAST)/PHAST                 CHANGE     81     I
RECO          GO TO 38                                                            CHANGE     82     I
RECO        37 HHRT(NNN) = HHRT(NNN) + C(IROW,I)*TP/(EX(I)+1.0)                   CHANGE     83     I
RECO          IF(EX(I).NE.0) GO TO 38                                             CHANGE     84     I
RECO          FC3 = FC3 + C(IROW,I)*ALOG(PHAST)                                   CHANGE     85     I
RECO          GO TO 32                                                            CHANGE     86     I
RECO        38 FC3 = FC3 + C(IROW,I)*TP/EX(I)                                     CHANGE     87     I
```

```
RECO        32 FC1 = FC1 = C(IROW,I)*TP                                          CHANGE     88     I
RECO           FHRT(NNN) = FC3 - HHRT(NNN)                                       CHANGE     89     I
RECO        45 CONTINUE                                                          CHANGE     90     I
RECO           IF (TEST(2)) CALL TAPEIN(LINES)                                   CHANGE     91     I
RECO           IOUT = 0                                          REC00102 RECO   105          D
RECO           IOUT = IBLNK                                                      CHANGE     92     I
RECO           GO TO 65                                          REC00156 RECO   157          D
RECO           HHRT(NTT) = HHRT(NTT) + ASDH/TT                                   CHANGE     93     I
RECO     C                                                                       CHANGE     94     I
RECO     C    CALCULATE CP/R FOR FIRST POINT AFTER PHASE TRANSITION USING UP TO A CHANGE     95     I
RECO     C    THREE POINT LAGRANGIAN INTERPOLATION WITH THE SECOND PHASE DATA.   CHANGE     96     I
RECO     C                                                                       CHANGE     97     I
RECO           IF(.NOT.TEST(2)) GO TO 34                                         CHANGE     98     I
RECO           IF(.NOT.TLAGR) GO TO 34                                           CHANGE     99     I
RECO           NLAGR = NLAGR + 1                                                 CHANGE    100     I
RECO           IF(NLAGR.EQ.1) TCONST = PHAST                                     CHANGE    101     I
RECO           IF(NLAGR.EQ.1) CPR(NNN) = CPR(NTT)                                CHANGE    102     I
RECO           IF(NLAGR.LT.2.OR.NLAGR.GT.3) GO TO 34                             CHANGE    103     I
RECO           CPR(NNN) = 0.0                                                    CHANGE    104     I
RECO           DO 35 K=1,NLAGR                                                   CHANGE    105     I
RECO           BK = 1.0                                                          CHANGE    106     I
RECO           NDEXK = NT - NLAGR + K                                            CHANGE    107     I
RECO           DO 36 J=1,NLAGR                                                   CHANGE    108     I
RECO           IF(J.EQ.K) GO TO 36                                               CHANGE    109     I
RECO           NDEXJ = NT - NLAGR + J                                            CHANGE    110     I
RECO           BK = BK*((PHAST-T(NDEXJ))/(T(NDEXK)-T(NDEXJ)))                    CHANGE    111     I
RECO        36 CONTINUE                                                          CHANGE    112     I
RECO           NDEXK = NTT-NLAGR + K                                             CHANGE    113     I
RECO           CPR(NNN) = CPR(NNN) + BK*CPR(NDEXK)                               CHANGE    114     I
RECO        35 CONTINUE                                                          CHANGE    115     I
RECO        34 CONTINUE                                                          CHANGE    116     I

ATOM           LOGICAL TEST,1STFIL,GLABEL                                        CHANGE    117     I
ATOM           EQUIVALENCE (Q,AJ),(TAPE,TDQDT)                                   CHANGE    118     I
ATOM           LOGICAL TEST,1STFIL,GLABEL                        ATOM0015 ATOM    22          D
ATOM           EQUIVALENCE (Q,AJ),(TAPE,TDQDT)                                   ATOM     23          D

LINK1          EQUIVALENCE (TAPE,SQ)                                             CHANGE    119     I
LINK1          EQUIVALENCE (TAPE,SQ)                                             LINK1     37          D

DERIV          DIMENSION I(5), J(6)                                              CHANGE    120     I
DERIV          DIMENSION I(5), J(6)                              DERI0009 DERIV   14          D

LEAST          NFP=NF                                                            CHANGE    121     I
LEAST          NPTS=NEND-NBEGIN+1                                                CHANGE    122     I
LEAST          NF=NFP                                                            CHANGE    123     I
LEAST          IF(NPTS.GE.NF) GO TO 47                                           CHANGE    124     I
```

```
LEAST          NF=NPTS                                                  CHANGE    125      I
LEAST       47 NF1=NF+1                                                 CHANGE    126      I
LEAST          NF2=NF+2                                                 CHANGE    127      I
LEAST          NF3=NF+3                                                 CHANGE    128      I
LEAST          NF4=NF+4                                                 CHANGE    129      I
LEAST          NF5=NF+5                                                 CHANGE    130      I
LEAST          NF6=NF+6                                                 CHANGE    131      I
LEAST          DO 49 I=NF1,NFP                                          CHANGE    132      I
LEAST       49 ANS(ILOW,I)=0.                                           CHANGE    133      I
LEAST          IF(T(L).LE.10000.)  GO TO 177                            LEAST     234        D
LEAST          IF(T(L).LE.10000.)  GO TO 510                            LEAST     247        D
LEAST      580 DO 581 I=1,NF5                                LEAS0309   LEAST     293        D
LEAST      580 DO 581 I=1,NF                                            CHANGE    134      I
LEAST          NFP1=NFP+1                                               CHANGE    135      I
LEAST          NFP2=NFP+2                                               CHANGE    136      I
LEAST          ANS(ILOW,NFP1)=ANSTPY(NF1)                               CHANGE    137      I
LEAST          ANS(ILOW,NFP2)=ANSTPY(NF2)                               CHANGE    138      I
LEAST          NFP = NF                                   LEAS0457      LEAST     444        D
LEAST          NF1=NFP1                                                 CHANGE    139      I
LEAST          NF2=NFP2                                                 CHANGE    140      I
LEAST          NF = NFP                                                 CHANGE    141      I


PUNCH          1       NLAST                                            PUNCH      19        D
PUNCH          1  NLAST, POLTLL, POLTUL                                 CHANGE    142      I
PUNCH           POLTLL = DAT4                                           CHANGE    143      I
PUNCH           POLTUL = DAT5                                           CHANGE    144      I

20

TAPIN     *DECK TAPIN                                                   TAPIN       1      I
TAPIN           SUBROUTINE TAPEIN(LINES)                                TAPIN       2      I
TAPIN     C                                                             TAPIN       3      I
TAPIN     C     INPUT FROM TAPE FOR METHOD READIN                       TAPIN       4      I
TAPIN     C                                                             TAPIN       5      I
TAPIN           LOGICAL TEST,IFIRST,NFRST                               TAPIN       6      I
TAPIN           DIMENSION NWC(8)                                        TAPIN       7      I
TAPIN           COMMON /TAP/IJW(800),T(100),DD(100,7),CHS(80),NREC,IFIRST  TAPIN    8      I
TAPIN           COMMON /INPT/TEST(20),ICARD,ICARD2,FWORD(4),IWORD(5),IWORD2(4),  TAPIN 9  I
TAPIN          1WORD(4),D(4),NAM(4),ITAPE                               TAPIN      10      I
TAPIN           DATA ARROW/6655555555555555555558/,AMINUS/1H-/          TAPIN      11      I
TAPIN           IOLDC = ICODE                                           TAPIN      12      I
TAPIN           READ (5,201) (NWC(I),I=1,8)                             TAPIN      13      I
TAPIN        201 FORMAT(8A10)                                           TAPIN      14      I
TAPIN           WRITE (6,202) (NWC(I),I=1,8)                            TAPIN      15      I
TAPIN        202 FORMAT(1H ,8A10/)                                      TAPIN      16      I
TAPIN           LINES = LINES + 2                                       TAPIN      17      I
TAPIN           IF(LINES.GE.55) CALL PAGEID(LINES)                      TAPIN      18      I
TAPIN           DECODE (80,203,NWC(1)) ICODE,TLL,TUL                    TAPIN      19      I
TAPIN        203 FORMAT(I4,2F4.0)                                       TAPIN      20      I
TAPIN           IF(ICODE.NE.IOLDC) IFIRST = .TRUE.                      TAPIN      21      I
TAPIN           IF(.NOT.IFIRST) GO TO 20                                TAPIN      22      I
TAPIN           IFIRST = .FALSE.                                        TAPIN      23      I
```

```
      BACKSPACE 8                                                        TAPIN      24      I
      IF (ICODE.LT.IOLDC) REWIND 8                                       TAPIN      25      I
      NREC = 0                                                           TAPIN      26      I
      IPAR = 0                                                           TAPIN      27      I
      NFRST = .TRUE.                                                     TAPIN      28      I
   19 BUFFER IN (8,0) (IJW(1),IJW(800))                                  TAPIN      29      I
      IF (UNIT(8))30,40,50                                               TAPIN      30      I
   30 CONTINUE                                                           TAPIN      31      I
      DO 10 M=1,100                                                      TAPIN      32      I
      N1 = 8*(M-1) + 1                                                   TAPIN      33      I
      DECODE (80,101,IJW(N1)) IKODE,(CHS(I),I=1,76)                      TAPIN      34      I
  101 FORMAT(I4,76A1)                                                    TAPIN      35      I
      IF(ICODE.EQ.IKODE) GO TO 204                                       TAPIN      36      I
      IF(NREC.LE.0) GO TO 10                                             TAPIN      37      I
      GO TO 20                                                           TAPIN      38      I
  204 IF(NFRST) GO TO 1000                                               TAPIN      39      I
      NREC = NREC + 1                                                    TAPIN      40      I
      IF(NREC.GT.100) GO TO 20                                           TAPIN      41      I
      DO 205 I=1,76                                                      TAPIN      42      I
      IF(CHS(I).EQ.ARROW) CHS(I) = AMINUS                                TAPIN      43      I
  205 CONTINUE                                                           TAPIN      44      I
      ENCODE(80,101,IJW(N1)) IKODE,(CHS(I),I=1,76)                       TAPIN      45      I
      WRITE(6,208) IKODE,(CHS(I),I=1,76)                                 TAPIN      46      I
  208 FORMAT(1H ,I4,76A1)                                                TAPIN      47      I
      LINES = LINES + 1                                                  TAPIN      48      I
      IF(LINES.GE.55) CALL PAGEID(LINES)                                 TAPIN      49      I
      DECODE(80,103,IJW(N1)) IKODE,T(NREC),(DD(NREC,K),K=1,3)            TAPIN      50      I
  103 FORMAT(I4,F4.0,F6.3,F10.0,2F10.3,3F10.0,6X)                        TAPIN      51      I
      IF(T(NREC).EQ.298.) T(NREC) = 298.15                               TAPIN      52      I
      GO TO 10                                                           TAPIN      53      I
 1000 NFRST = .FALSE.                                                    TAPIN      54      I
   10 CONTINUE                                                           TAPIN      55      I
      GO TO 19                                                           TAPIN      56      I
   40 WRITE (6,458)                                                      TAPIN      57      I
  458 FORMAT (30H EOF ENCOUNTERED ON INPUT TAPE)                         TAPIN      58      I
      LINES = LINES + 1                                                  TAPIN      59      I
      IF(LINES.GE.55) CALL PAGEID(LINES)                                 TAPIN      60      I
      GO TO 20                                                           TAPIN      61      I
   50 WRITE (6,459)                                                      TAPIN      62      I
  459 FORMAT (27H PARITY ERROR ON INPUT TAPE)                            TAPIN      63      I
      LINES = LINES + 1                                                  TAPIN      64      I
      IF(LINES.GE.55) CALL PAGEID(LINES)                                 TAPIN      65      I
      IPAR=IPAR + 1                                                      TAPIN      66      I
      IF (IPAR.GT.20) GO TO 20                                           TAPIN      67      I
      GO TO 19                                                           TAPIN      68      I
   20 CONTINUE                                                           TAPIN      69      I
      REWIND 4                                                           TAPIN      70      I
      IF(NREC.GT.100) NREC = 100                                         TAPIN      71      I
      ITAPE=0                                                            TAPIN      72      I
      DO 206 I=1,NREC                                                    TAPIN      73      I
      IF(T(I).LT.TLL.OR.T(I).GT.TUL) GO TO 206                           TAPIN      74      I
      ITAPE = ITAPE + 1                                                  TAPIN      75      I
      WRITE(4,207) T(I),DD(I,1),DD(I,3),DD(I,2)                          TAPIN      76      I
  207 FORMAT(4HDATA,2X,1HT,5X,F12.2,2HCP,4X,F12.3,1HS,5X,F12.3,4HM-H2,   TAPIN      77      I
     1  2X,F12.0,2X)                                                    TAPIN      78      I
```

```
TAPIN      206 CONTINUE                                    TAPIN       79      I
TAPIN          REWIND 4                                    TAPIN       80      I
TAPIN          RETURN                                      TAPIN       81      I
TAPIN          END                                         TAPIN       82      I
```

CORRECTION IDENTS ARE LISTED IN CHRONOLOGICAL ORDER OF INSERTION

MAIN	INPUT	PAGEID	EFTAPE	IDENT	TEMPER	RECO	ATOM
POLY	LINK1	DERIV	QSUM	DELH	TABLES	LEAST	LOGK
PUNCH	BLOCK	CHANGE	TAPIN				

DECKS ARE LISTED IN THE ORDER OF THEIR OCCURRENCE ON A NEW PROGRAM LIBRARY IF ONE IS CREATED BY THIS UPDATE

YANK$$$	MAIN	INPUT	PAGEID	EFTAPE	IDENT	TEMPER	RECO
ATOM	POLY	LINK1	DERIV	QSUM	DELH	TABLES	LEAST
LOGK	PUNCH	BLOCK	TAPIN				

DECKS WRITTEN TO COMPILE FILE

MAIN	INPUT	PAGEID	EFTAPE	IDENT	TEMPER	RECO	ATOM
POLY	LINK1	DERIV	QSUM	DELH	TABLES	LEAST	LOGK
PUNCH	BLOCK	TAPIN					

THIS UPDATE REQUIRED 34200B WORDS OF CORE.

APPENDIX C

Example

Input

```
NA201(S)                ASINDH -99900.
LSTSQS
METHODREADIN            MELTPT 1405.2
 373 3001023
METHODREADIN            DELTAH 420.     T     1023.2
 37310231243
METHODREADIN            DELTAH 2850.    T     1243.2
 37312431405
METHODREADIN            DELTAH 11400.   T     1405.2      ASINDH-89112.
 37414053000
FINISH
STOP
```

OUTPUT

```
NA201(S)                ASINUM -99900.                                  0

LSTSW.S                                                                 0

METHODREADIN            MELTPT 1405.2                                   0
 373 3001023

 373   0     0      -2964         0  INFINITE    -98744    -98744  INFINITE   668
 373 100  7828      -2685      3979     30827    -99452    -96642    211212   668
 373 200 14233      -1525     11761     19387    -99815    -93655    102341   668
 373 298 16516          0     17935     17935    -99900    -90609     66418   668
 373 300 16550         31     18038     17936    -99900    -90550     65966   668
 373 400 18111       1765     23017     18604   -101209    -87329     47714   668
 373 500 19478       3648     27212     19917   -101174    -83858     36654   668
 373 600 20485       5648     30856     21443   -100993    -80410     29289   668
 373 700 21236       7735     34073     23022   -100707    -77003     24041   668
 373 800 21819       9889     36948     24586   -100342    -73640     20118   668
 373 900 22291      12095     39546     26106    -99923    -70327     17078   668
3731000 22666      14345     41915     27570    -99467    -67062     14656   668
3731100 23029      17051     44504     29004    -98572    -63879     12692   668
3731200 23334      19369     46521     30380   -144558    -59832     10897   668
3731300 23611      24567     50693     31795   -140783    -52938      8900   668
3731400 23867      26941     52452     33209   -139835    -46217      7215   668
3731500 24108      29339     54107     34547   -138866    -39564      5764   668
3731600 24336      31762     55670     35819   -137876    -32975      4504   668
3731700 24554      34206     57152     37031   -136864    -26448      3400   668
3731800 24765      36672     58561     38188   -135837    -19983      2426   668
3731900 24969      39159     59906     39296   -134792    -13574      1561   668
3732000 25169      41666     61192     40359   -133731     -7224       789   668

DATA  T          300.00CP          16.550S          18.038M-M2          31.  0

DATA  T          400.00CP          18.111S          23.017M-M2        1765.  0

DATA  T          500.00CP          19.478S          27.212M-M2        3648.  0

DATA  T          600.00CP          20.485S          30.856M-M2        5648.  0

DATA  T          700.00CP          21.236S          34.073M-M2        7735.  0

DATA  T          800.00CP          21.819S          36.948M-M2        9889.  0

DATA  T          900.00CP          22.291S          39.546M-M2       12095.  0

DATA  T         1000.00CP          22.686S          41.915M-M2       14345.  0

METHODREADIN            DELTAH 420.       T      1023.2                  0
```


NA201(S)

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-FH/RT INPUT INPUT-CALC	-FH/RT CALC FRACTION
300.00	8.3284478	8.3239285	.0520004	.0509261	9.0772533	9.0756628	9.0252529	9.0247367
	.0045194	.0005426	.0010743	.0206588	.0015905	.0001752	.0005162	.0000572
400.00	9.1139890	9.1282914	2.2205001	2.2227041	11.5828328	11.5838895	9.3623328	9.3611854
	-.0143024	-.0015693	-.0022040	-.0009926	-.0010567	-.0000912	.0011474	.0001226
500.00	9.8019037	9.7876421	3.6715623	3.6721799	13.6938805	13.6943396	10.0223182	10.0221596
	.0142616	.0014550	-.0006177	-.0001682	-.0004591	-.0000335	.0001586	.0000158
600.00	10.3086558	10.3053028	4.7370668	4.7364578	15.5276487	15.5266671	10.7905819	10.7902093
	.0033530	.0003253	.0006090	.0001286	.0009816	.0000632	.0003726	.0000345
700.00	10.6865811	10.6957605	5.5606857	5.5612829	17.1465379	17.1460535	11.5858522	11.5847706
	-.0091794	-.0008590	-.0005972	-.0001074	.0004844	.0000283	.0010816	.0000934
800.00	10.9799639	10.9846676	6.2205453	6.2220367	18.5933226	18.5940815	12.3727773	12.3720449
	-.0047037	-.0004284	-.0014913	-.0002397	-.0007589	-.0000408	.0007324	.0000592
900.00	11.2174882	11.2088413	6.7628450	6.7640682	19.9007128	19.9012526	13.1378678	13.1371844
	.0086469	.0007708	-.0012232	-.0001809	-.0005398	-.0000271	.0006834	.0000520
1000.00	11.4162639	11.4162639	7.2188268	7.2188268	21.0928635	21.0928635	13.8740366	13.8740366
	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000

MAX-REL ERR CP/R = .001569 TEMP = 400. AVER REL ERR CP/R = .000744 REL LST SQ ERR CP/R = .000901
MAX REL ERR HH/RT = .020659 TEMP = 300. AVER REL ERR HH/RT = .002810 REL LST SQ ERR HH/RT = .007314
MAX REL ERR S/R = .000175 TEMP = 300. AVER REL ERR S/R = .000057 REL LST SQ ERR S/R = .000077
MAX REL ERR FH/RT = .000123 TEMP = 400. AVER REL ERR FH/RT = .000054 REL LST SQ ERR FH/RT = .000066
MAX ERR CP/R = .014302 TEMP = 400. AVER ERR CP/R = .007371 LST SQ ERR CP/R = .008809
MAX ERR HH/RT = .002204 TEMP = 400. AVER ERR HH/RT = .000977 LST SQ ERR HH/RT = .001164
MAX ERR S/R = .001591 TEMP = 300. AVER ERR S/R = .000734 LST SQ ERR S/R = .000860
MAX ERR FH/RT = .001147 TEMP = 400. AVER ERR FH/RT = .000587 LST SQ ERR FH/RT = .000700

CP/R = 5.1750201E+00T** 0.0 1.1788277E-02T** 1.0 -2.3790507E-06T** 2.0 -7.8200767E-09T** 3.0 4.6520945E-12T** 4.0

(H-H0)/R CONSTANT = -.20327145E+04, H/R(A6) CONSTANT = -.52305339E+05, S/R CONSTANT = -.23809992E+02

```
NA20(S)                NA  20   1    0    0S   300.000  1000.000            1
 0.            0.              0.             0.                           2
 0.            0.               .51750201E+01  .11788277E-01 -.23790507E-05 3
-.78200767E-08  .46520945E-11 -.52305339E+05 -.23809992E+02                 4
```


NA201(S)

37310231243

DATA T	1100.00CP	23.029S	44.504M-M2	17051. 0
DATA T	1200.00CP	23.334S	46.521M-M2	19369. 0
METHODREADIN	DELTAH 2850.	T	1243.2	0

NA201(S)

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HM/RT INPUT INPUT-CALC	HM/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-FM/RT INPUT INPUT-CALC	-FM/RT CALC FRACTION
1023.20	11.4709951	11.4709951	7.5211456	7.5211456	21.5618458	21.5618458	14.0407002	14.0407002
	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000
1100.00	11.5888716	11.5887223	7.8005143	7.8010254	22.3957246	22.3962691	14.5952102	14.5952436
	.0001492	.0000129	-.0005111	-.0000655	-.0005445	-.0000243	-.0000334	-.0000023
1200.00	11.7423566	11.7423307	8.1225431	8.1230647	23.4107384	23.4112031	15.2881953	15.2881384
	.0000258	.0000022	-.0005216	-.0000642	-.0004647	-.0000198	.0000569	.0000037

MAX-REL ERR CP/R = .000013 TEMP = 1100. AVER REL ERR CP/R = .000005 REL LST SQ ERR CP/R = .000006
MAX REL ERR HM/RT = .000066 TEMP = 1100. AVER REL ERR HM/RT = .000043 REL LST SQ ERR HM/RT = .000053
MAX REL ERR S/R = .000024 TEMP = 1100. AVER REL ERR S/R = .000015 REL LST SQ ERR S/R = .000018
MAX REL ERR FM/RT = .000004 TEMP = 1200. AVER REL ERR FM/RT = .000002 REL LST SQ ERR FM/RT = .000003
MAX ERR CP/R = .000149 TEMP = 1100. AVER ERR CP/R = .000058 LST SQ ERR CP/R = .000087
MAX ERR HM/RT = .000522 TEMP = 1200. AVER ERR HM/RT = .000344 LST SQ ERR HM/RT = .000422
MAX ERR S/R = .000545 TEMP = 1100. AVER ERR S/R = .000336 LST SQ ERR S/R = .000413
MAX ERR FM/RT = .000057 TEMP = 1200. AVER ERR FM/RT = .000030 LST SQ ERR FM/RT = .000038

CP/R = 9.9227516E+00T** 0.0 1.4947509E-03T** 1.0 1.7970868E-08T** 2.0
(H-H0)/R CONSTANT = -.32461962E+04, H/R(A6) CONSTANT = -.53518821E+05, S/R CONSTANT = -.48748509E+02

```
NA20(S)                    NA  20    1     0     0S  1023.200  1200.000            1
  .99227516E+01  .14947509E-02  .17970868E-07 0.              0.                  2
 -.53518821E+05 -.48748509E+02 0.             0.              0.                  3
 0.             0.             0.             0.                                  4
```


NA201(S)

```
3731243140S

DATA  T          1300.00CP          23.611S          50.693M-M2          24567.  0
DATA  T          1400.00CP          23.867S          52.452M-M2          26941.  0
METHODREADIN              DELTAH 11400.     T     1405.2     ASINDH-89112.      0
```


NA201(S)

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-FH/RT INPUT INPUT-CALC	-FH/RT CALC FRACTION
1243.20	11.8085775	11.8085775	9.4036244	9.4036244	24.9813031	24.9813031	15.5776787	15.5776787
	0.0000000	0.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000
1300.00	11.8817511	11.8816765	9.5098758	9.5102990	25.5102118	25.5104784	16.0003360	16.0001794
	.0000746	.0000063	-.0004232	-.0000445	-.0002666	-.0000105	.0001566	.0000098
1400.00	12.0105779	12.0105606	9.6839324	9.6842847	26.3953924	26.3957205	16.7114601	16.7114359
	.0000173	.0000014	-.0003523	-.0000364	-.0003281	-.0000124	.0000242	.0000014

MAX-REL ERR CP/R =	.000006	TEMP =	1300.	AVER REL ERR CP/R =	.000003	REL LST SQ ERR CP/R =	.000004
MAX REL ERR HH/RT =	.000045	TEMP =	1300.	AVER REL ERR HH/RT =	.000027	REL LST SQ ERR HH/RT =	.000033
MAX REL ERR S/R =	.000012	TEMP =	1400.	AVER REL ERR S/R =	.000008	REL LST SQ ERR S/R =	.000009
MAX REL ERR FH/RT =	.000010	TEMP =	1300.	AVER REL ERR FH/RT =	.000004	REL LST SQ ERR FH/RT =	.000006
MAX ERR CP/R =	.000075	TEMP =	1300.	AVER ERR CP/R =	.000031	LST SQ ERR CP/R =	.000044
MAX ERR HH/RT =	.000423	TEMP =	1300.	AVER ERR HH/RT =	.000259	LST SQ ERR HH/RT =	.000318
MAX ERR S/R =	.000328	TEMP =	1400.	AVER ERR S/R =	.000198	LST SQ ERR S/R =	.000244
MAX ERR FH/RT =	.000157	TEMP =	1300.	AVER ERR FH/RT =	.000060	LST SQ ERR FH/RT =	.000091

CP/R = 1.0228080E+01T** 0.0 1.2563579E-03T** 1.0 1.2030588E-08T** 2.0

(H-H0)/R CONSTANT = -.20035476E+04, H/R(A6) CONSTANT = -.52276172E+05, S/R CONSTANT = -.49469506E+02

NA20(S) NA 20 1 0 0S 1243.200 1400.000

.10228080E+02	.12563579E-02	.12030588E-07	0.	0.	1
-.52276172E+05	-.49469506E+02	0.	0.	0.	2
0.	0.	0.	0.		3
					4

NA201(S)

3741405 3000

374 298 25000	0	21895	21895	-89112	-81001	59376	668
374 300 25000	46	22050	21895	-89096	-80950	58972	668
374 400 25000	2546	29242	22876	-89640	-78249	42753	668
374 500 25000	5046	34820	24728	-88987	-75476	32990	668
374 600 25000	7546	39378	26801	-88307	-72837	26531	668
374 700 25000	10046	43232	28880	-87608	-70316	21954	668
374 800 25000	12546	46570	30887	-86897	-67893	18548	668
374 900 25000	15046	49515	32797	-86184	-65560	15920	668
3741000 25000	17546	52149	34603	-85477	-63306	13836	668
3741100 25000	20046	54532	36308	-84789	-61126	12145	668
3741200 25000	22546	56707	37918	-130593	-58089	10579	668
3741300 25000	25046	58708	39442	-129515	-52090	8757	668
3741400 25000	27546	60561	40885	-128441	-46176	7208	668
3741500 25000	30046	62286	42255	-127371	-40337	5877	668
3741600 25000	32546	63899	43558	-126303	-34569	4722	668
3741700 25000	35046	65415	44799	-125236	-28867	3711	668
3741800 25000	37546	66844	45985	-124175	-23229	2820	668
3741900 25000	40046	68195	47118	-123116	-17649	2030	668
3742000 25000	42546	69478	48204	-122062	-12127	1325	668
3742100 25000	45046	70697	49247	-121009	-6658	693	668
3742200 25000	47546	71860	50248	-119961	-1236	123	668
3742300 25000	50046	72972	51212	-118915	4135	-393	668
3742400 25000	52546	74036	52141	-117874	9466	-862	668
3742500 25000	55046	75056	53038	-116836	14746	-1289	668
3742600 25000	57546	76037	53903	-115804	19993	-1681	668
3742700 25000	60046	76980	54741	-114777	25194	-2039	668
3742800 25000	62546	77889	55551	-113756	30357	-2369	668
3742900 25000	65046	78767	56337	-112740	35491	-2675	668
3743000 25000	67546	79614	57099	-111733	40584	-2957	668

DATA T	1500.00CP	25.000S	62.286M-M2	30046. 0
DATA T	1600.00CP	25.000S	63.899M-M2	32546. 0
DATA T	1700.00CP	25.000S	65.415M-M2	35046. 0
DATA T	1800.00CP	25.000S	66.844M-M2	37546. 0
DATA T	1900.00CP	25.000S	68.195M-M2	40046. 0
DATA T	2000.00CP	25.000S	69.478M-M2	42546. 0
DATA T	2100.00CP	25.000S	70.697M-M2	45046. 0
DATA T	2200.00CP	25.000S	71.860M-M2	47546. 0
DATA T	2300.00CP	25.000S	72.972M-M2	50046. 0
DATA T	2400.00CP	25.000S	74.036M-M2	52546. 0

NA201(S)

NA201(S)

DATA	T	2500.00CP	25.000S	75.056M-M2	55046. 0
DATA	T	2600.00CP	25.000S	76.037M-M2	57546. 0
DATA	T	2700.00CP	25.000S	76.980M-M2	60046. 0
DATA	T	2800.00CP	25.000S	77.889M-M2	62546. 0
DATA	T	2900.00CP	25.000S	78.767M-M2	65046. 0
DATA	T	3000.00CP	25.000S	79.614M-M2	67546. 0
FINISH					0

NA201(S)

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HM/RT INPUT INPUT-CALC	HM/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-FM/RT INPUT INPUT-CALC	-FM/RT CALC FRACTION
1400.20	12.5807369	12.5807369	13.7754675	13.7754675	30.5228229	30.5228229	16.7473554	16.7473554
	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000
1500.00	12.5807369	12.5805214	13.6992483	13.6999531	31.3441511	31.3441546	17.6449028	17.6442015
	.0002154	.0000171	-.0007048	-.0000515	-.0000035	-.0000001	.0007013	.0000397
1600.00	12.5807369	12.5804031	13.6293413	13.6299844	32.1558602	32.1560785	18.5265189	18.5260941
	.0003338	.0000265	-.0006431	-.0000472	-.0002183	-.0000068	.0004248	.0000224
1700.00	12.5807369	12.5803664	13.5676587	13.5682429	32.9187561	32.9187593	19.3510974	19.3505164
	.0003705	.0000294	-.0005842	-.0000431	-.0000032	-.0000001	.0005811	.0000300
1800.00	12.5807369	12.5803847	13.5128297	13.5133612	33.6378710	33.6378334	20.1250413	20.1244722
	.0003521	.0000280	-.0005315	-.0000393	.0000377	.0000011	.0005692	.0000283
1900.00	12.5807369	12.5804355	13.4637722	13.4642584	34.3177341	34.3180211	20.8539619	20.8537627
	.0003014	.0000240	-.0004862	-.0000361	-.0002870	-.0000084	.0001992	.0000096
2000.00	12.5807369	12.5805003	13.4196204	13.4200689	34.9633775	34.9633147	21.5437571	21.5432454
	.0002366	.0000188	-.0004485	-.0000334	.0000628	.0000018	.0005112	.0000237
2100.00	12.5807369	12.5805646	13.3796736	13.3800910	35.5768142	35.5771209	22.1971406	22.1970300
	.0001723	.0000137	-.0004174	-.0000312	-.0003067	-.0000086	.0001106	.0000050
2200.00	12.5807369	12.5806182	13.3433583	13.3437501	36.1620701	36.1623703	22.8187118	22.8186202
	.0001186	.0000094	-.0003919	-.0000294	-.0003002	-.0000083	.0000916	.0000040
2300.00	12.5807369	12.5806550	13.3102008	13.3105714	36.7216613	36.7216018	23.4114604	23.4110305
	.0000819	.0000065	-.0003705	-.0000278	.0000594	.0000016	.0004300	.0000184
2400.00	12.5807369	12.5806727	13.2798065	13.2801586	37.2570974	37.2570301	23.9772909	23.9768715
	.0000642	.0000051	-.0003521	-.0000265	.0000673	.0000018	.0004194	.0000175
2500.00	12.5807369	12.5806734	13.2518437	13.2521792	37.7703915	37.7705983	24.5185478	24.5184191
	.0000635	.0000050	-.0003355	-.0000253	-.0002068	-.0000055	.0001287	.0000052
2600.00	12.5807369	12.5806631	13.2260319	13.2263519	38.2640596	38.2640211	25.0380277	25.0376692
	.0000738	.0000059	-.0003200	-.0000242	.0000385	.0000010	.0003585	.0000143
2700.00	12.5807369	12.5806519	13.2021321	13.2024373	38.7386050	38.7388192	25.5364729	25.5363820
	.0000849	.0000068	-.0003052	-.0000231	-.0002142	-.0000055	.0000909	.0000036
2800.00	12.5807369	12.5806543	13.1799394	13.1802306	39.1960406	39.1963479	26.0161012	26.0161173
	.0000826	.0000066	-.0002912	-.0000221	-.0003073	-.0000078	-.0000161	-.0000065
2900.00	12.5807369	12.5806883	13.1592772	13.1595561	39.6378761	39.6378201	26.4785988	26.4782641
	.0000486	.0000039	-.0002788	-.0000212	.0000559	.0000014	.0003348	.0000126
3000.00	12.5807369	12.5807766	13.1399926	13.1402617	40.0641114	40.0643263	26.9241189	26.9240645
	-.0000397	-.0000032	-.0002692	-.0000205	-.0002148	-.0000054	.0000543	.0000020

MAX-REL ERR CP/R = .000029 TEMP = 1700.
MAX REL ERR HM/RT = .000051 TEMP = 1500.
MAX REL ERR S/R = .000009 TEMP = 2100.
MAX REL ERR FM/RT = .000040 TEMP = 1500.
MAX ERR CP/R = .000370 TEMP = 1700.
MAX ERR HM/RT = .000705 TEMP = 1500.
MAX ERR S/R = .000307 TEMP = 2800.
MAX ERR FM/RT = .000701 TEMP = 1500.

AVER REL ERR CP/R = .000012
AVER REL ERR HM/RT = .000030
AVER REL ERR S/R = .000004
AVER REL ERR FM/RT = .000014
AVER ERR CP/R = .000155
AVER ERR HM/RT = .000396
AVER ERR S/R = .000140
AVER ERR FM/RT = .000295

REL LST SQ ERR CP/R = .000016
REL LST SQ ERR HM/RT = .000032
REL LST SQ ERR S/R = .000005
REL LST SQ ERR FM/RT = .000018
LST SQ ERR CP/R = .000195
LST SQ ERR HM/RT = .000427
LST SQ ERR S/R = .000182
LST SQ ERR FM/RT = .000367

CP/R = 1.2622733E+01T** 0.0 -7.8387249E-05T** 1.0 5.3196078E-08T** 2.0 -1.5688274E-11T** 3.0 1.7040059E-15T** 4.0

NA201(S)

NA201(S)

```
(H-H0)/R CONSTANT =    .16614384E+04, H/R(A6) CONSTANT = -.48611186E+05, S/R CONSTANT = -.60895442E+02

NA20(L)
                    NA   20    1     0     0L  1405.200  3000.000                    1
 .12622733E+02 -.78387249E-04  .53196078E-07 -.15688274E-10  .17040059E-14          2
-.48611186E+05 -.60895442E+02 0.             0.             0.                     3
 0.             0.            0.             0.                                    4
```


NA201(S)

NA201(S)

H298 = -99900.000

T	CP/R	(H-H0)/RT	(H-H298)/RT	S/R	-(G-H0)/RT	-(G-H298)/RT	H/RT	-G/RT
300.00	8.3284478	.0520004		9.0772533	9.0252529		-147.5234148	156.6006681
400.00	9.1139890	2.2205001		11.5828328	9.3623328		-123.4610614	135.0438942
500.00	9.8019037	3.6715623		13.6938805	10.0223182		-96.8736869	110.5675674
600.00	10.3086558	4.7370668		15.5276487	10.7905819		-79.0506408	94.5782895
700.00	10.6865811	5.5606857		17.1465379	11.5858522		-66.2573494	83.4038873
800.00	10.9799639	6.2205453		18.5933226	12.3727773		-56.6202354	75.2135540
900.00	11.2174882	6.7628450		19.9007128	13.1378678		-49.0956267	68.9963336
1000.00	11.4162639	7.2188268		21.0928635	13.8740366		-43.0537977	64.1466612
1023.20	11.4709951	7.5211456		21.5618458	14.0407002		-41.6115993	63.1734451
1100.00	11.5888716	7.8005143		22.3957246	14.5952102		-37.9018716	60.2975962
1200.00	11.7423566	8.1225431		23.4107384	15.2881953		-33.7713107	57.1820491
1243.20	11.8085775	9.4036244		24.9813031	15.5776787		-31.0344584	56.0157615
1300.00	11.8817511	9.5098758		25.5102118	16.0003360		-29.1613739	54.6715857
1400.00	12.0105779	9.6839324		26.3953924	16.7114601		-26.2250852	52.6204776
1405.20	12.5807369	13.7754675		30.5228229	16.7473554		-22.0006673	52.5234902
1500.00	12.5807369	13.6992483		31.3441511	17.6449028		-19.8158348	51.1599859
1600.00	12.5807369	13.6293413		32.1558602	18.5265189		-17.7910491	49.9469093
1700.00	12.5807369	13.5676587		32.9187561	19.3510974		-16.0044734	48.9232295
1800.00	12.5807369	13.5128297		33.6378710	20.1250413		-14.4164062	48.0542772
1900.00	12.5807369	13.4637722		34.3177341	20.8539619		-12.9955039	47.3132380
2000.00	12.5807369	13.4196204		34.9633775	21.5437571		-11.7166919	46.6800693
2100.00	12.5807369	13.3796736		35.5768142	22.1971406		-10.5596715	46.1364857
2200.00	12.5807369	13.3433583		36.1620701	22.8187118		-9.5078347	45.6699048
2300.00	12.5807369	13.3102008		36.7216613	23.4114604		-8.5474620	45.2691233
2400.00	12.5807369	13.2798065		37.2570974	23.9772909		-7.6671204	44.9242178
2500.00	12.5807369	13.2518437		37.7703915	24.5185478		-6.8572061	44.6275976
2600.00	12.5807369	13.2260319		38.2640596	25.0380277		-6.1095929	44.3736525
2700.00	12.5807369	13.2021321		38.7386050	25.5364729		-5.4173585	44.1559635
2800.00	12.5807369	13.1799394		39.1960406	26.0161012		-4.7745694	43.9706100
2900.00	12.5807369	13.1592772		39.6378761	26.4785988		-4.1761105	43.8139866
3000.00	12.5807369	13.1399926		40.0641114	26.9241189		-3.6175490	43.6816604

NA201(S)

H298 = -99900.000

T	CP	H-H0	H-H298	S	-(G-H0)	-(G-H298)	H	-G
300.00	16.5500000	31.0000		18.036000	5380.4000		-99869.0000	105280.4000
400.00	18.1110000	1765.0000		23.017000	7441.8000		-98135.0000	107341.8000
500.00	19.4780000	3648.0000		27.212000	9958.0000		-96252.0000	109858.0000
600.00	20.4850000	5648.0000		30.856000	12865.6000		-94252.0000	112765.6000
700.00	21.2360000	7735.0000		34.073000	16116.1000		-92165.0000	116016.1000
800.00	21.8190000	9889.0000		36.948000	19669.4000		-90011.0000	119569.4000
900.00	22.2910000	12095.0000		39.546000	23496.4000		-87805.0000	123396.4000
1000.00	22.6860000	14345.0000		41.915000	27570.0000		-85555.0000	127470.0000
1023.20	22.7947600	15292.4989		42.846945	28548.4956		-84607.5011	128448.4956
1100.00	23.0290000	17051.0000		44.504000	31903.4000		-82849.0000	131803.4000
1200.00	23.3340000	19369.0000		46.521000	36456.2000		-80531.0000	136356.2000
1243.20	23.4655920	20231.1230		49.641971	38483.7756		-76668.8770	138383.7756
1300.00	23.6110000	24567.0000		50.693000	41333.9000		-75333.0000	141233.9000
1400.00	23.8670000	26941.0000		52.452000	46491.8000		-72959.0000	146391.8000
1405.20	25.0000000	38466.1230		60.653885	46764.7167		-61433.8770	146664.7167
1500.00	25.0000000	40834.0000		62.286000	52595.0000		-59066.0000	152495.0000
1600.00	25.0000000	43334.0000		63.899000	58904.4000		-56566.0000	158804.4000
1700.00	25.0000000	45834.0000		65.415000	65371.5000		-54066.0000	165271.5000
1800.00	25.0000000	48334.0000		66.844000	71985.2000		-51566.0000	171885.2000
1900.00	25.0000000	50834.0000		68.195000	78736.5000		-49066.0000	178636.5000
2000.00	25.0000000	53334.0000		69.478000	85622.0000		-46566.0000	185522.0000
2100.00	25.0000000	55834.0000		70.697000	92629.7000		-44066.0000	192529.7000
2200.00	25.0000000	58334.0000		71.860000	99758.0000		-41566.0000	199658.0000
2300.00	25.0000000	60834.0000		72.972000	107001.6000		-39066.0000	206901.6000
2400.00	25.0000000	63334.0000		74.036000	114352.4000		-36566.0000	214252.4000
2500.00	25.0000000	65834.0000		75.056000	121806.0000		-34066.0000	221706.0000
2600.00	25.0000000	68334.0000		76.037000	129362.2000		-31566.0000	229262.2000
2700.00	25.0000000	70834.0000		76.980000	137012.0000		-29066.0000	236912.0000
2800.00	25.0000000	73334.0000		77.889000	144755.2000		-26566.0000	244655.2000
2900.00	25.0000000	75834.0000		78.767000	152590.3000		-24066.0000	252490.3000
3000.00	25.0000000	78334.0000		79.614000	160508.0000		-21566.0000	260408.0000

NA201(S)

```
NA2O(S)                 NA   2O    1    0    0S   300.000  1000.000*          1
 0.              0.              0.              0.              0.            2
 0.              0.               .51750201E+01   .11788277E-01 -.23790507E-05 3
-.78200767E-08   .46520945E-11 -.52305334E+05  -.23809992E+02                 4
NA2O(S)                 NA   2O    1    0    0S  1023.200  1200.000*          1
 .99227516E+01   .14947509E-02   .17970868E-07  0.              0.            2
-.53518821E+05  -.48748509E+02   0.              0.              0.            3
 0.              0.              0.              0.                            4
NA2O(S)                 NA   2O    1    0    0S  1243.200  1400.000*          1
 .10228080E+02   .12563579E-02   .12030588E-07  0.              0.            2
-.52276172E+05  -.49469506E+02   0.              0.              0.            3
 0.              0.              0.              0.                            4
NA2O(L)                 NA   2O    1    0    0L  1405.200  3000.000           1
 .12022733E+02  -.78347249E-04   .53196078E-07 -.15688274E-10   .17040059E-14 2
-.48611186E+05  -.60895442E+02   0.              0.              0.            3
 0.              0.              0.              0.                            4
```

*For input as data to the NASA thermodynamics program[3], these temperatures should be manually corrected to match the lower limits of the next higher range; i.e., 1023.2, 1243.2, and 1405.2, respectively. The problem is only with the printout. The thermodynamic quantities calculated from the polynomial coefficients listed here are consistent at the transition temperatures.

-In the particular example presented here, the lowest range has a transition less than 100° above 1000K. The seven coefficients listed were computed for the entire range 300-1023K, and must therefore be copied into the first seven places, where now zeros appear.

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